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Atmospheric Chemistry and Physics Discussions

Interactive comment on "SIMPOL.1: A simple group contribution method for predicting vapor pressures and enthalpies of vaporization of multifunctional organic compounds" *by* J. F. Pankow and W. E. Asher

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Responses to Reviewers of ACPD-2007-0285, Pankow and Asher: SIMPOL.1: A Simple Group Contribution Method for Predicting Vapor Pressures and Enthalpies of Vaporization of Multifunctional Organic Compounds

Reviewer #2

Specific Comment #1: It would probably be worthwhile to mention in the conclusions that besides the inherent uncertainties in the vapor pressures estimated using this method, gas-particle partitioning is also affected by the activity coefficient of the com-

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pound in a particular matrix.

Response: We agree with Reviewer #2 that activities are important for modeling gas-particle partitioning. However, this topic is far too complex and too important to do justice to in a few sentences in the conclusions of this paper. We feel it is better to restrict the conclusions to only the SIMPOL.1 parameterization of vapor pressure. Future work in this area by ourselves will undoubtedly explore this issue. We will defer discussion of the relative roles of uncertainty in pLo and activity coefficients in aerosol modeling until that time.

Technical Comment #1. Page 11846, first paragraph: Since logP decreases by˜-0.5 for each carbon number, P decreases by ˜1/3 of an order of magnitude (i.e., a factor of ˜3). This is much different than 1/2 of an order of magnitude when applied to a long carbon chain. This relation is one that is easy to remember (as a rule of thumb), so the value should be stated accurately.

Response: Corrected. Thank you for catching the error.

Technical Comment #2. Table 6, superscript d: This should be primary, secondary, and tertiary nitrate group, not nitro group.

Response: Corrected. Thank you for catching the error.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 11839, 2007.